

# SUMMARY

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## Nuclear Data - Cross Section & Covariances - For GNEP and AFC

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# Basis for our priorities

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- Salvatores' presentation on GNEP/AFC and R&D needs
- Areas where DOE/Science research can make an impact
- DOE Science is the owner of the ENDF library & related infrastructure
- Technical discussions at this workshop



# Highest Priority: Covariances (WG A's highest priority)

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- Clear need from reactor design & AFC community
  - To compare target uncertainties provided by reactor design community (&WPEC), with our estimates of current uncertainties
  - (We have specialized expertise in understanding nuclear data uncertainties, based on cross section measurements, theory predictions, and a knowledge of integral experiments)
  - Sensitivity calculations with our covariances will help focus future work (exp, theory, data evaluations)
  - This builds on recent breakthroughs in new methodologies for evaluating covariances; US playing a co-leading role internationally.
- We propose:
  - Global (though somewhat crude) assessment for all nuclei in ENDF/B-VII.0; create initial new library - end of CY07  
Upgrades to our processing codes (NJOY etc) to process covariances
  - 08-09: Provide refined covariances for priority materials, esp actinides and minor actinides, for ENDF/B-VII.1.(Progress already here)
  - FY10-15. Produce new ENDF/B-VII.2 for broad suite of isotopes



# Rest ... not in any particular priority ordering:

## Major actinides

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- **Improve poor thermal and intermediate  $^{239}\text{Pu}$  criticality.** Much ENDF/B-VII data testing points to weaknesses in  $^{239}\text{Pu}$  data in the thermal (and possibly intermediate) region –  $k$ -eff are overpredicted significantly. Although there are very fast assemblies (eg Jezebel) that indicate our cross sections perform well in the high energy region, there are very few lower energy more intermediate assemblies involving  $^{239}\text{Pu}$ . The one or two in the ICSBEP benchmark book in the intermediate region are also largely overpredicted. This suggests that for GNEP plans involving fast reactors with significant  $^{239}\text{Pu}$  content, an improved  $^{239}\text{Pu}$  evaluation is needed – possibly in the resolved and unresolved resonance regions.
- $^{239}\text{Pu}(n,g)$ . Salvatores noted that  $^{239}\text{Pu}(n,g)$  is needed to less than 8 % above about 1 keV; Our current covariance analysis (Kawano at LANL) provides covariance uncertainties of ~10-15% in this range, so more work is needed.
- $^{235}\text{U}(n,g)$ . 10% uncertainties ~ 100 keV should be resolved; Inelastic scattering needs a modern re-evaluation to fix a problem that seems to be leading to neutron spectra in HEU that are too soft. Mikey Bradey noted related concerns.



## Other issues... not in any particular priority ordering:

### Minor actinides

**Americium data improvements.**  $^{242}\text{mAm}$  fission and capture need further improvements. The target uncertainties from Salvatores were significantly smaller than our current uncertainties, even with the recent evaluation work at LANL for this isotope. Future work should build upon the LANL and BNL reaction calculations, and on future planned measurements of capture & fission at the DANCE detector, using LLNL's target. The  $^{241}\text{Am}$  capture reaction was also of priority from Salvatores, and the target uncertainty he provided ( $\sim 10\%$ ) requires additional modeling and experimental work. Finally, we note that  $(n,2n)$  cross sections on actinides require new data (eg for  $^{241}\text{Am}(n,2n)$  and  $^{243}\text{Am}(n,2n)$ , especially for the region just above the  $n2n$  threshold (say 5.5-11 MeV), since this region is important when folded with a fission neutron spectrum, for impacting transmutation rates up and down an isotope chain.

- **Curium data improvements.**  $^{244}, ^{245}\text{Cm}$  data uncertainties appear to be important, according to Salvatores's report (though we didn't see target uncertainties in his report). These isotopes have been ignored, to date, in the US community in recent years. Future improved evaluations, especially of capture and fission and inelastic scattering, may be needed.



## Other issues... not in any particular priority ordering:

### Reaction modeling codes

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- Tools developed in our community for nuclear reaction modeling, for predicting cross sections, are fairly sophisticated but need to be improved
- GNASH, EMPIRE, KALMAN, COH, ...
  - Continue collaborate with international community to advance these tools (eg Koning TALYS, Bruyeres-le-Chatel, Caderache, ....)
  - Utilize new more fundamental capabilities being developed eg new SCIDAC colaboration
  - Use new experiments where available to improve models
- Fission modeling improvements are a priority
  - Esp. for unmeasured cases, or cases where data are sparse (eg  $^{242}\text{mAm}$ )



## Other issues... not in any particular priority ordering:

### ~~Decay Data, Delayed Neutrons, Photon Production~~

- Decay Data. New BNL evaluation in ENDF/B-VII will require additional upgrades for AFC/GNEP needs
- Delayed neutrons. AFC/GNEP have pointed to some upgrades needed - 6-group representations, spectra, modifications at thermal,...
- Photon production. Most ENDF evaluations have very poor production and spectra representations.
  - GNEP/AFC noted various improvements needed
  - We can build upon advances in our modeling codes recently developed (eg recently demonstrated for Ge, and oil-well logging applications)
  - DANCE type experiments could help



# Future Vision ....GNDI for GNEP!

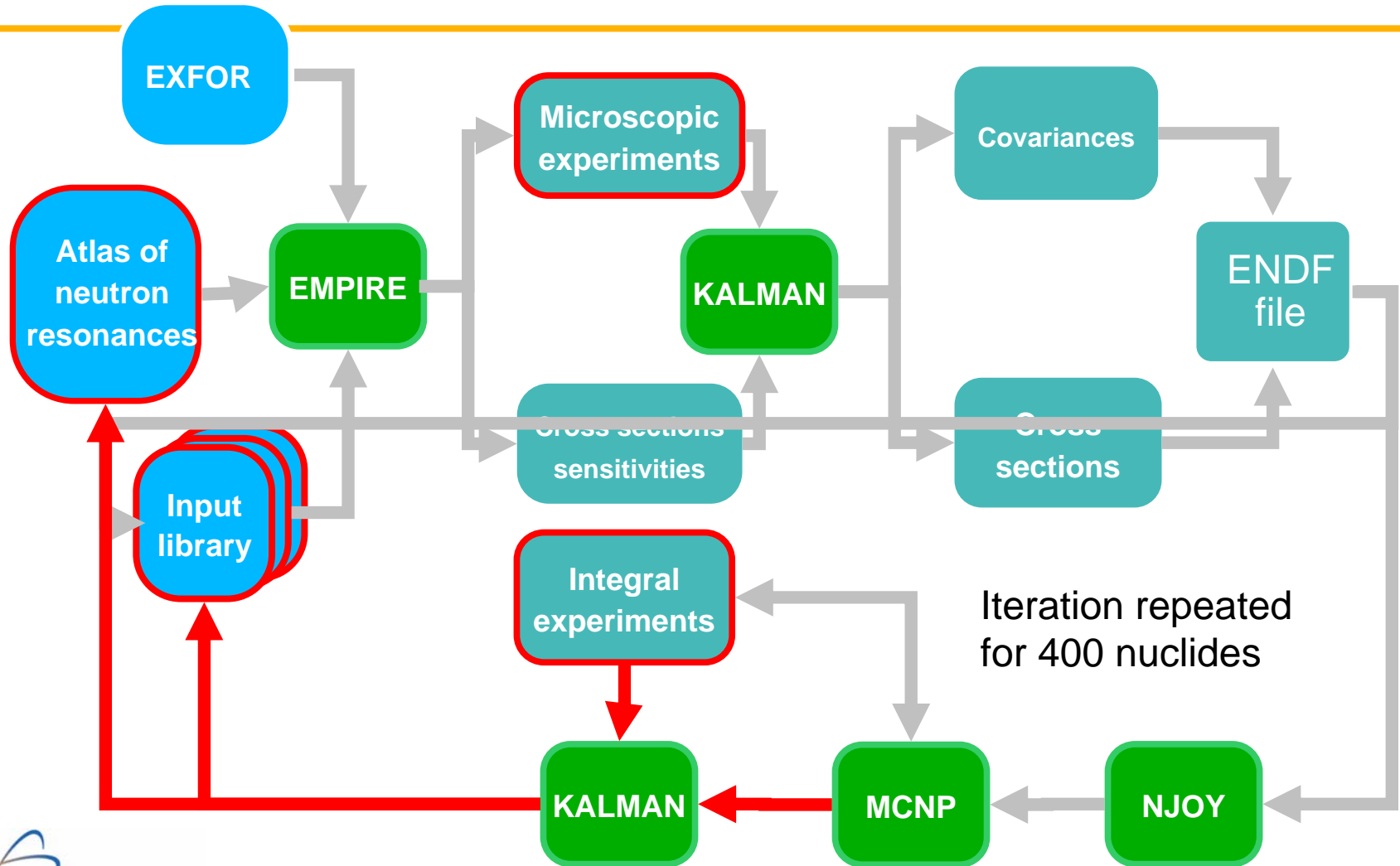
## High-Performance Computation and Simulation

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- A completely different way of thinking about nuclear data evaluation for GNEP/AFC
- Automated approach to optimize input modeling parameters to match
  - Fundamental cross section data
  - Integral criticality data and other well constrained benchmarks
  - Automatically generate covariances
- Builds on tools recently developed, and new simulation and HPC opportunities



# Global Nuclear Data Initiative





# CPU time estimate

- Assumptions (for single 3GHz PC):
  - 400 nuclides
  - 50 parameters/nuclide
  - Single model calculation (1 nuclide up to 20 MeV) – 20 min
  - benchmark sensitivity to a single parameter 500 min
  - full library benchmark 400 000 min
- Single iteration (min):
  - Model calculations:  
 $400 \times 50 \times 2 \times 20 = 800\,000$
  - Benchmark parameter-sensitivity:  
 $400 \times 50 \times 2 \times 500 = 20\,000\,000$
  - Library benchmarking:  
400 000
  - Total:  
 $\sim 21\,000\,000 \text{ min} = 40 \text{ years}$
- 1 iteration per week - 2100 CPU's